Glutaric acid, (2-chlorocyclohexyl)methyl but-3-yn-2-yl ester

Inchi: InChI=1S/C16H23ClO4/c1-3-12(2)21-16(19)10-6-9-15(18)20-11-13-7-4-5-8-14(13)17/h1,

InchiKey: GSHXLKDRXZKNSM-UHFFFAOYSA-N

Formula: C16H23ClO4

SMILES: C#CC(C)OC(=O)CCCC(=O)OCC1CCCCC1Cl

Mol. weight [g/mol]: 314.80

Physical Properties

Property code	Value	Unit	Source
gf	-158.56	kJ/mol	Joback Method
hf	-558.31	kJ/mol	Joback Method
hfus	39.32	kJ/mol	Joback Method
hvap	73.50	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.062		Crippen Method
mcvol	243.960	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	2166.00		NIST Webbook
rinpol	2166.00		NIST Webbook
tb	760.05	K	Joback Method
tc	972.23	K	Joback Method
tf	479.43	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.85	J/mol×K	760.05	Joback Method
cpg	727.86	J/mol×K	795.41	Joback Method
cpg	743.63	J/mol×K	830.78	Joback Method
cpg	758.20	J/mol×K	866.14	Joback Method
cpg	771.58	J/mol×K	901.50	Joback Method
cpg	783.78	J/mol×K	936.86	Joback Method
cpg	794.82	J/mol×K	972.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume